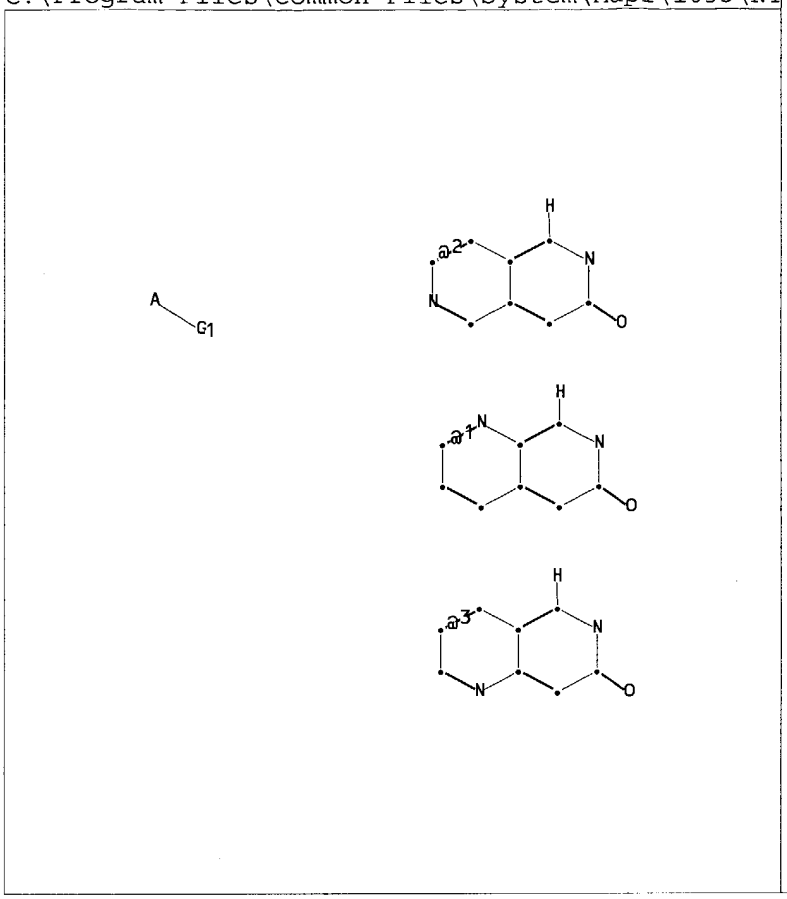
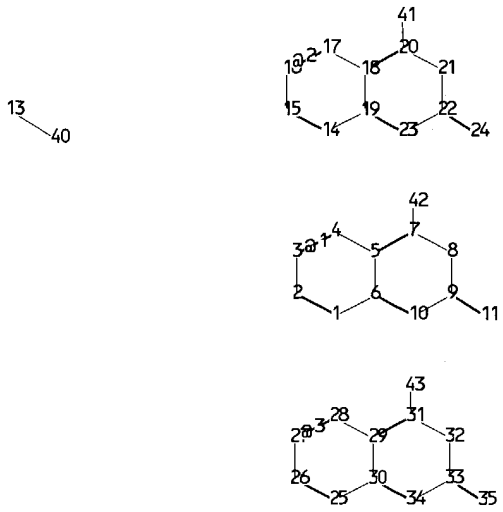
L Number	Hits	Search Text	DB	Time stamp
1	752	(546/141).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/03/19 11:37
2	1939	((514/300) or (514/309) or (546/122) or (546/123)).CCLS.	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/03/19 11:46
3	2427	((546/141).CCLS.) or (((514/300) or (514/309) or (546/122) or (546/123)).CCLS.)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2004/03/19 11:46

C:\Program Files\Common Files\System\Mapi\1033\NT






```
chain nodes :
    11  24  35  40  41  42  43
ring nodes :
    1  2  3  4  5  6  7  8  9  10  14  15  16  17  18  19  20  21  22  23  25  26  27  28  29
    30  31  32  33  34
ring/chain nodes :
    13
chain bonds :
    7-42  9-11  13-40  20-41  22-24  31-43  33-35
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  14-15  14-19  15-16  16-17  17-18
    18-19  18-20  19-23  20-21  21-22  22-23  25-26  25-30  26-27  27-28  28-29  29-30  29-31
    30-34  31-32  32-33  33-34
exact/norm bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-40  14-15  14-19  15-16
    16-17  17-18  18-19  18-20  19-23  20-21  21-22  22-23  22-24  25-26  25-30  26-27  27-28
    28-29  29-30  29-31  30-34  31-32  32-33  33-34  33-35
exact bonds :
    7-42  20-41  31-43
isolated ring systems :
    containing 1 : 14 : 25 :


G1:[*1],[*2],[*3]

Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom  11:CLASS
    13:CLASS  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:Atom  22:Atom
    23:Atom  24:CLASS  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:Atom  32:Atom
    33:Atom  34:Atom  35:CLASS  40:CLASS  41:CLASS  42:CLASS  43:CLASS
```

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

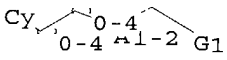
L1 SCREEN CREATED

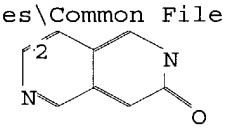
=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

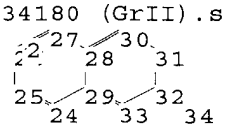
L2 SCREEN CREATED

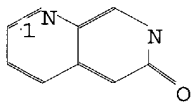
=>

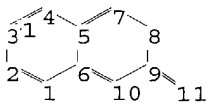
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (GrII).str

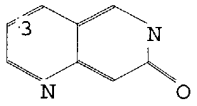


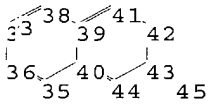












chain nodes :
11 13 14 15 20 21 34 45 50
ring nodes :
1 2 3 4 5 6 7 8 9 10 24 25 26 27 28 29 30 31 32 33 35 36 37 38 39 40 41 42 43 44
chain bonds :
9-11 13-14 13-50 14-15 15-20 20-21 32-34 43-45
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 24-25 24-29 25-26 26-27 27-28 28-29 28-30 29-33 30-31 31-32 32-33 35-36 35-40 36-37 37-38 38-39 39-40 39-41 40-44 41-42 42-43 43-44

```
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-14  13-50  14-15
20-21  24-25  24-29  25-26  26-27  27-28  28-29  28-30  29-33  30-31  31-32  32-33
32-34  35-36  35-40  36-37  37-38  38-39  39-40  39-41  40-44  41-42  42-43  43-44
43-45
exact bonds :
15-20
isolated ring systems :
containing 1 : 24 : 35 :


G1:[*1],[*2],[*3]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  13:CLASS  14:CLASS  15:CLASS  20:CLASS  21:Atom  24:Atom  25:Atom
26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  33:Atom  34:CLASS
35:Atom  36:Atom  37:Atom  38:Atom  39:Atom  40:Atom  41:Atom  42:Atom  43:Atom
44:Atom  45:CLASS  50:CLASS



L3      STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4   QUE L3 AND L1 NOT L2

=> d l4
L4 HAS NO ANSWERS
L1              SCR 1839
L2              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L3              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L4              QUE  L3 AND L1 NOT L2


=> s l4 sss sam
SAMPLE SEARCH INITIATED 13:13:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   7875 TO ITERATE

 12.7% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       152183 TO   162817
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L3 AND L1 NOT L2

=> s l4 sss ful
FULL SEARCH INITIATED 13:13:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 159266 TO ITERATE
```

100.0% PROCESSED 159266 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.05

L6 0 SEA SSS FUL L3 AND L1 NOT L2

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

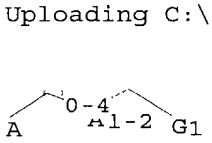
=> screen 1839

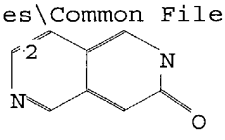
L7 SCREEN CREATED

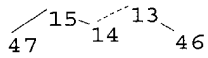
=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

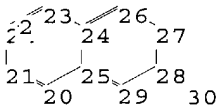
L8 SCREEN CREATED

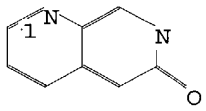
=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (GrIIa).str

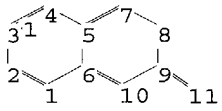


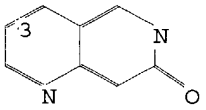


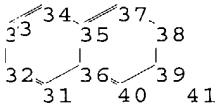












chain nodes :
11 13 14 15 30 41 46
ring nodes :
1 2 3 4 5 6 7 8 9 10 20 21 22 23 24 25 26 27 28 29 31 32 33
34 35 36 37 38 39 40

```
ring/chain nodes :
47
chain bonds :
9-11  13-14  13-46  14-15  15-47  28-30  39-41
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  20-21  20-25  21-22  22-23
 23-24  24-25  24-26  25-29  26-27  27-28  28-29  31-32  31-36  32-33  33-34  34-35
 35-36  35-37  36-40  37-38  38-39  39-40
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-14  13-46  14-15
15-47  20-21  20-25  21-22  22-23  23-24  24-25  24-26  25-29  26-27  27-28  28-29
28-30  31-32  31-36  32-33  33-34  34-35  35-36  35-37  36-40  37-38  38-39  39-40
39-41
isolated ring systems :
containing 1 : 20 : 31 :


G1:[*1],[*2],[*3]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  13:CLASS  14:CLASS  15:CLASS  20:Atom  21:Atom  22:Atom  23:Atom  24:Atom
 25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:CLASS  31:Atom  32:Atom  33:Atom
34:Atom  35:Atom  36:Atom  37:Atom  38:Atom  39:Atom  40:Atom  41:CLASS  46:CLASS
47:CLASS



L9      STRUCTURE UPLOADED

=> que L9 AND L7 NOT L8

L10  QUE L9 AND L7 NOT L8

=> d l10
L10 HAS NO ANSWERS
L7              SCR 1839
L8              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L9              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L10             QUE  L9 AND L7 NOT L8


=> s l10 sss sam
SAMPLE SEARCH INITIATED 13:14:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   7875 TO ITERATE

 12.7% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       152183 TO   162817
PROJECTED ANSWERS:               0 TO        0
```

L11 0 SEA SSS SAM L9 AND L7 NOT L8

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

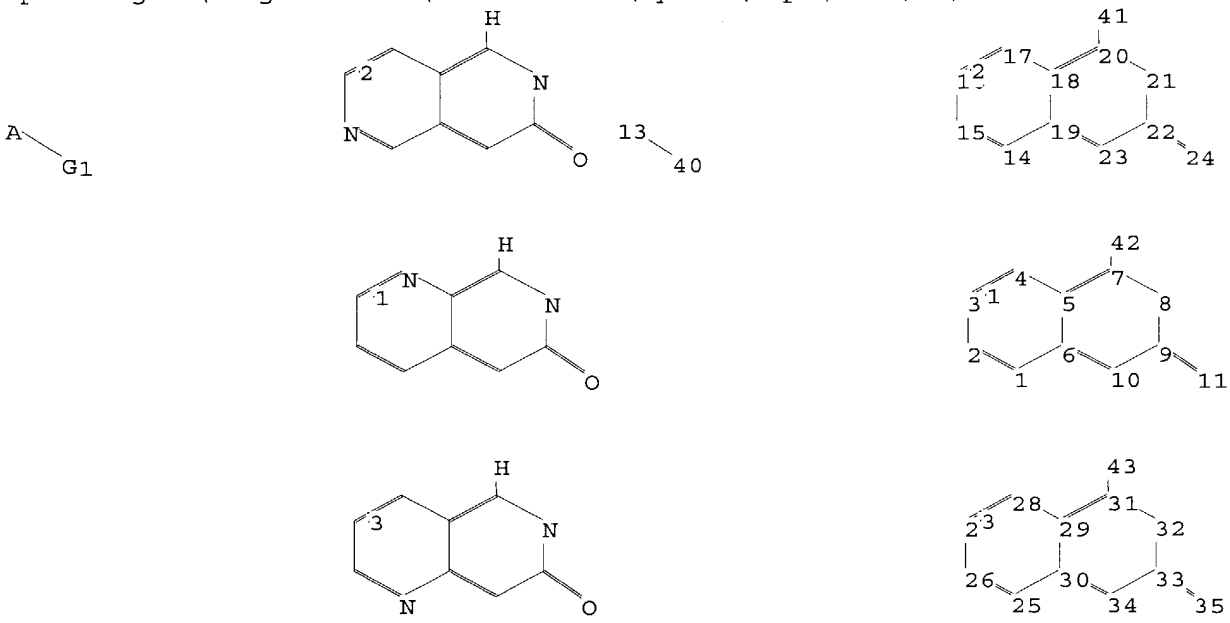
L12 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L13 SCREEN CREATED

=>

Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (GrIIb).str



chain nodes :
11 24 35 40 41 42 43
ring nodes :
1 2 3 4 5 6 7 8 9 10 14 15 16 17 18 19 20 21 22 23 25 26 27
28 29 30 31 32 33 34

```
ring/chain nodes :
13
chain bonds :
7-42  9-11  13-40  20-41  22-24  31-43  33-35
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  14-15  14-19  15-16  16-17
 17-18  18-19  18-20  19-23  20-21  21-22  22-23  25-26  25-30  26-27  27-28  28-29
 29-30  29-31  30-34  31-32  32-33  33-34
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-40  14-15  14-19
15-16  16-17  17-18  18-19  18-20  19-23  20-21  21-22  22-23  22-24  25-26  25-30
26-27  27-28  28-29  29-30  29-31  30-34  31-32  32-33  33-34  33-35
exact bonds :
7-42  20-41  31-43
isolated ring systems :
containing 1 : 14 : 25 :


G1:[*1],[*2],[*3]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  13:CLASS  14:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom
21:Atom  22:Atom  23:Atom  24:CLASS  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom
30:Atom  31:Atom  32:Atom  33:Atom  34:Atom  35:CLASS  40:CLASS  41:CLASS  42:CLASS
 43:CLASS



L14      STRUCTURE UPLOADED

=> que L14 AND L12 NOT L13

L15  QUE L14 AND L12 NOT L13

=> d l15
L15 HAS NO ANSWERS
L12              SCR 1839
L13              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L14              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L15              QUE  L14 AND L12 NOT L13


=> s l15 sss sam
SAMPLE SEARCH INITIATED 13:17:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   9618 TO ITERATE

 10.4% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       186485 TO   198235
PROJECTED ANSWERS:               0 TO        0
```

```
L16             0 SEA SSS SAM L14 AND L12 NOT L13

=> s l15 sss ful
FULL SEARCH INITIATED 13:18:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 193946 TO ITERATE

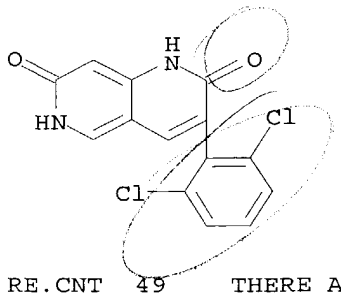
100.0% PROCESSED  193946 ITERATIONS                                 7 ANSWERS
SEARCH TIME: 00.00.04

L17             7 SEA SSS FUL L14 AND L12 NOT L13

=> => s l17
L18             4 L17

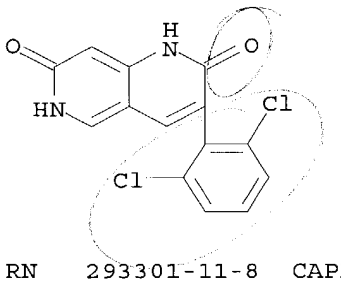
=> d l18 1-4 bib,ab,hitstr
```

L18 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:473076 CAPLUS
DN 133:252336
TI Synthesis and Structure-Activity Relationships of 7-Substituted 3-(2,6-Dichlorophenyl)-1,6-naphthyridin-2(1H)-ones as Selective Inhibitors of pp60c-src
AU Thompson, Andrew M.; Rewcastle, Gordon W.; Boushelle, Stacey L.; Hartl, Brian G.; Kraker, Alan J.; Lu, Gina H.; Batley, Brian L.; Panek, Robert L.; Showalter, H. D. Hollis; Denny, William A.
CS Auckland Cancer Society Research Centre Faculty of Medical and Health Sciences, University of Auckland, Auckland, 92019, N. Z.
SO Journal of Medicinal Chemistry (2000), 43(16), 3134-3147
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB 7-Substituted 3-(2,6-dichlorophenyl)-1,6-naphthyridin-2(1H)-ones are potent inhibitors of protein tyrosine kinases, with some selectivity for c-Src. The compds. were prepared by condensing 4,6-diaminonicotinaldehyde with 2,6-dichlorophenylacetonitrile and selectively converting the 2- and 7-amino groups of the product to hydroxy and fluoro groups, resp., by prolonged diazotization in 50% aqueous fluoroboric acid. N-Methylation, followed by treatment with aliphatic diamines, aromatic amines, or their derived lithium anions, gave the desired compds. Selected isomeric 1,8-naphthyridin-2(1H)-ones were also prepared in order to evaluate the relative contributions of both ring A aza atoms of the related pyrido[2,3-d]pyrimidin-7(8H)-ones to the inhibitory activity. The compds. were evaluated for their ability to prevent phosphorylation of a model substrate by c-Src, FGF-1 receptor, and PDGF-β receptor enzymes. Overall, there was a high degree of correlation of the activities against the different kinases, with c-Src being generally the most sensitive to structural changes. 1,6-Naphthyridin-2(1H)-one analogs bearing basic aliphatic side chains [7-NH(CH2)nNRR, 7-NHC6H4O(CH2)nNRR, or 7-NHC6H4N(CH2)4NMe] were the most potent against c-Src (IC50s of 10-80 nM), showing good selectivity with respect to PDGFR (10-300-fold) but less with respect to FGFR. The 1,6-naphthyridin-2(1H)-ones showed broadly similar activity to the analogous pyrido[2,3-d]pyrimidin-7(8H)-ones, whereas the 1,8-naphthyridin-2(1H)-ones were at least 103-fold less potent. These results, indicating that the 3-aza atom in the pyrido[2,3-d]pyrimidin-7(8H)-ones is mandatory, whereas the 1-aza atom is not, support the published binding model for these compds. to c-Src (J. Med. Chemical 1998, 41, 1752), where the 3-aza and 2-NH atoms form a bidentate H-bond donor-acceptor motif that interacts with Met341 and the 1-aza atom is not involved in specific binding interactions.
IT **220822-19-5P**
RL: BYP (Byproduct); PREP (Preparation)
(preparation and structure-activity relationships of 7-substituted 3-(2,6-Dichlorophenyl)-1,6-naphthyridin-2(1H)-ones as selective inhibitors of pp60c-src)
RN 220822-19-5 CAPLUS
CN 1,6-Naphthyridine-2,7(1H,6H)-dione, 3-(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

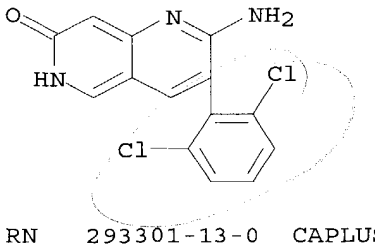


RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:386062 CAPLUS
DN 133:252283
TI Synthesis of 7-substituted 3-aryl-1,6-naphthyridin-2-amines and 7-substituted 3-aryl-1,6-naphthyridin-2(1H)-ones via diazotization of 3-aryl-1,6-naphthyridine-2,7-diamines
AU Thompson, Andrew M.; Showalter, H. D. Hollis; Denny, William A.
CS Faculty of Medical and Health Sciences, Auckland Cancer Society Research Centre, The University of Auckland, Auckland, N. Z.
SO Perkin 1 (2000), (12), 1843-1852
CODEN: PERKF9
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 133:252283
AB The preparation of 3-aryl-7-halo-1,6-naphthyridin-2-amines and 3-aryl-7-halo-1,6-naphthyridin-2(1H)-ones from the diazotization of 3-aryl-1,6-naphthyridine-2,7-diamines is reported. The reactions were investigated in various solvents (concentrated HCl, 50% HBF4, 70% HF-pyridine, 20% and 90% H2SO4, dilute HCl, and neat TFA). By appropriate choice of solvent and other conditions, good yields of the target compds. could be obtained, although in some cases a variety of different side products was also produced. Subsequent displacement of the 7-halogen substituents with alkylamines provides a route to more complex 7-substituted 1,6-naphthyridine derivs. that are potential tyrosine kinase inhibitors.
IT **220822-19-5P 293301-11-8P 293301-13-0P**
293301-15-2P 293301-28-7P 293304-90-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 220822-19-5 CAPLUS
CN 1,6-Naphthyridine-2,7(1H,6H)-dione, 3-(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

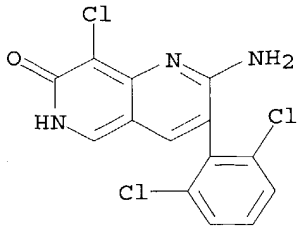


RN 293301-11-8 CAPLUS
CN 1,6-Naphthyridin-7(6H)-one, 2-amino-3-(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)

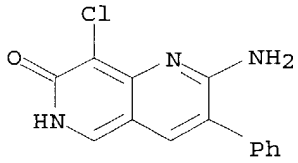


RN 293301-13-0 CAPLUS
CN 1,6-Naphthyridin-7(6H)-one, 2-amino-8-chloro-3-(2,6-dichlorophenyl)- (9CI)

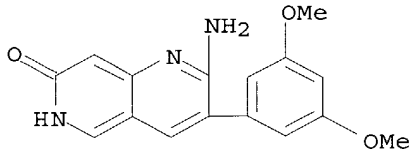
(CA INDEX NAME)



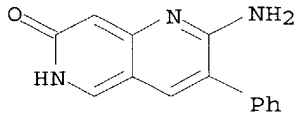
RN 293301-15-2 CAPLUS
CN 1,6-Naphthyridin-7(6H)-one, 2-amino-8-chloro-3-phenyl- (9CI) (CA INDEX NAME)



RN 293301-28-7 CAPLUS
CN 1,6-Naphthyridin-7(6H)-one, 2-amino-3-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 293304-90-2 CAPLUS
CN 1,6-Naphthyridin-7(6H)-one, 2-amino-3-phenyl- (9CI) (CA INDEX NAME)

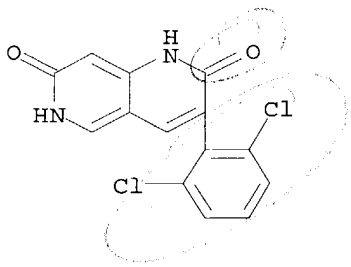


RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:139846 CAPLUS
DN 130:196643
TI Preparation of naphthyridinones as protein tyrosine kinase and cyclin dependant kinase inhibitors
IN Barvian, Mark Robert; Denny, William Alexander; Dobrusin, Ellen Myra; Hamby, James Marino; Showalter, Howard Daniel Hollis; Thompson, Andrew Mark; Winters, Roy Thomas; Wu, Zhipei
PA Warner-Lambert Company, USA
SO PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

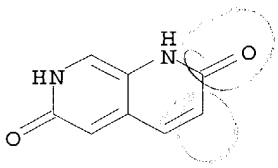
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9909030	A1	19990225	WO 1998-US16848	19980813
	W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9888289	A1	19990308	AU 1998-88289	19980813
	AU 742999	B2	20020117		
	EP 1003745	A1	20000531	EP 1998-939941	19980813
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 9811956	A	20000815	BR 1998-11956	19980813
	JP 2001515078	T2	20010918	JP 2000-509710	19980813
	NZ 502704	A	20020628	NZ 1998-502704	19980813
	ZA 9807491	A	19990421	ZA 1998-7491	19980819
	MX 9911792	A	20000630	MX 1999-11792	19991215
	US 6150359	A	20001121	US 2000-463553	20000126
PRAI	US 1997-56746P	P	19970820		
	WO 1998-US16848	W	19980813		

OS MARPAT 130:196643
AB Title compds. [I; R1 = halo or (un)substituted amino; R2 = (bi)(cyclo)alkyl; R5 = H, halo, (hetero)aryl, etc.; dashed line = optional bond] were prepared Thus, 4,6-diamino-3-pyridinecarboxaldehyde (preparation given) was cyclocondensed with 2,6-Cl2C6H3CH2CN and the major product treated with NaNO2/HBF4 to give, after N-methylation, major product I (R2 = Me, R5 = C6H3Cl2-2,6)(II; R1 = F) which was aminated to give II (R1 = e.g., NHMe). Data for biol. activity of I were given.
IT **220822-19-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of naphthyridinones as protein tyrosine kinase and cyclin dependant kinase inhibitors)
RN 220822-19-5 CAPLUS
CN 1,6-Naphthyridine-2,7(1H,6H)-dione, 3-(2,6-dichlorophenyl)- (9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:76356 CAPLUS
DN 74:76356
TI Synthesis of substituted 1,5- and 1,7-naphthyridines and related lactams
AU Rapoport, Henry; Frydman, Benjamin; Los, Mario
CS Univ. California, Berkeley, CA, USA
SO Journal of Organic Chemistry (1971), 36(3), 450-4
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 74:76356
AB Reductive cyclization of Et 2-methoxy-5-nitro-4-pyridinepyruvate and of Et 6-methoxy-3-nitro-2-pyridinepyruvate afforded the corresponding 1,2,3,4-tetrahydro-3-oxy-6-methoxy-1,7-naphthyridin-2-one and 1,2,3,4-tetrahydro-3-oxy-6-methoxy-1,5-naphthyridin-2-one. Treatment of the latter with p-toluenesulfonyl chloride in pyridine afforded 6-methoxy-1,7-naphthyridin-2(1H)-one and 6-methoxy-1,5-naphthyridin-2(1H)-one, which by treatment with POCl3 were transformed into 2-chloro-6-methoxy-1,7-naphthyridine, 2-chloro-6-methoxy-1,5-naphthyridine, and 2,6-dichloro-1,5-naphthyridine. The 2-chloronaphthyridines were transformed into 2-hydrazinonaphthyridines and reduced with Cu2+ to the parent naphthyridines. 2-Chloro-1,5-naphthyridine afforded 2-methoxy-1,5-naphthyridine by mild treatment with NaOMe. Hydrogenation of 6-methoxy-1,7-naphthyridin-2(1H)-one afforded 1,2,3,4-tetrahydro-6-methoxy-1,7-naphthyridin-2-one. Treatment of 6-methoxy-1,7-naphthyridin-2(1H)-one and its 1,5 analog with HBr afforded the 1,2,6,7-tetrahydro-1,7-naphthyridine-2,6-dione and 1,2,6,7-tetrahydro-1,5-naphthyridine-2,6-dione, which were reduced to the cis-decahydro-1,7- and -1,5-naphthyridine-2,6-diones. The bicyclic lactams could not be hydrolyzed to the amino acids, which were prepared by acid hydrolysis of meso- and rac-2,2'-bi(pyrrolidine)-5,5'-dione. When the di-Et meso- and rac-4,5-diaminosuberate dihydrochlorides were equilibrated at pH 7.5, they cyclized to the six-membered bicyclic lactams, trans- and cis-decahydro-1,5-naphthyridine-2,6-dione, resp.
IT **27017-62-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 27017-62-5 CAPLUS
CN 1,7-Naphthyridine-2,6-dione, 1,7-dihydro- (8CI) (CA INDEX NAME)



```
=> => d his

     (FILE 'HOME' ENTERED AT 13:12:32 ON 19 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 13:12:36 ON 19 MAR 2004
L1                SCREEN 1839
L2                SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L3                STRUCTURE UPLOADED
L4                QUE L3 AND L1 NOT L2
L5              0 S L4 SSS SAM
L6              0 S L4 SSS FUL
L7                SCREEN 1839
L8                SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L9                STRUCTURE UPLOADED
L10               QUE L9 AND L7 NOT L8
L11             0 S L10 SSS SAM
L12               SCREEN 1839
L13               SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L14               STRUCTURE UPLOADED
L15               QUE L14 AND L12 NOT L13
L16             0 S L15 SSS SAM
L17             7 S L15 SSS FUL

     FILE 'CAPLUS' ENTERED AT 13:18:10 ON 19 MAR 2004
L18             4 S L17

     FILE 'CAOLD' ENTERED AT 13:18:34 ON 19 MAR 2004

=> s l17
L19           0 L17

=> log y
COST IN U.S. DOLLARS                            SINCE FILE       TOTAL
                                                  ENTRY     SESSION
FULL ESTIMATED COST                                0.42      333.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE       TOTAL
                                                  ENTRY     SESSION
CA SUBSCRIBER PRICE                                0.00       -2.77

STN INTERNATIONAL LOGOFF AT 13:18:48 ON 19 MAR 2004
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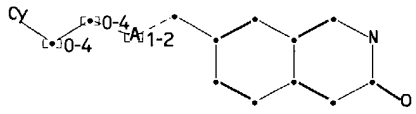
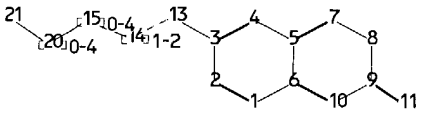
C:\Program Files\Common Files\System\Mapi\1033\NT





chain nodes :
    11 13 14 15 20 21
ring nodes :
    1 2 3 4 5 6 7 8 9 10
chain bonds :
    3-13 9-11 13-14 14-15 15-20 20-21
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-11 13-14 14-15 20-21
exact bonds :
    3-13 15-20
isolated ring systems :
    containing 1 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS
    13:CLASS 14:CLASS 15:CLASS 20:CLASS 21:Atom

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

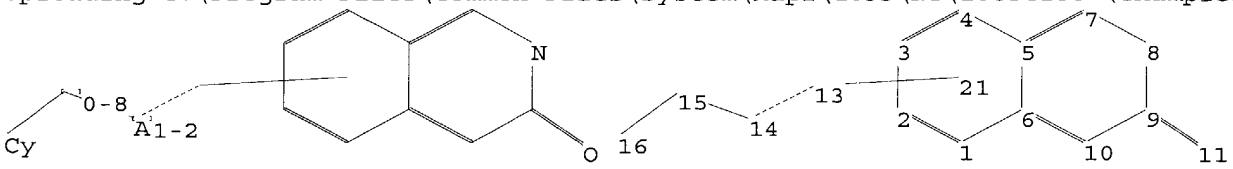

=> screen 1839

L1     SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L2     SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (examples).str
```




```
chain nodes :
11  13  14  15  16
ring nodes :
1  2  3  4  5  6  7  8  9  10
chain bonds :
9-11  13-14  14-15  15-16
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-14  14-15  15-16
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  13:CLASS  14:CLASS  15:CLASS  16:Atom  21:CLASS

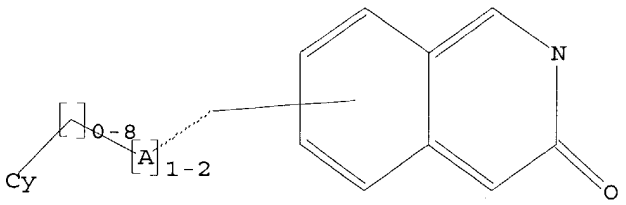


L3      STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4   QUE L3 AND L1 NOT L2

=> d l4
L4 HAS NO ANSWERS
L1              SCR 1839
L2              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L3              STR
```



Structure attributes must be viewed using STN Express query preparation.
L4 QUE L3 AND L1 NOT L2

=> s l4 sss sam
SAMPLE SEARCH INITIATED 11:01:58 FILE 'REGISTRY'

SEARCH INTERRUPTED

L5 QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> s l4 sss sam
SAMPLE SEARCH INITIATED 11:02:12 FILE 'REGISTRY'

SEARCH INTERRUPTED

L6 QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> s l4 sss sam
SAMPLE SEARCH INITIATED 11:02:43 FILE 'REGISTRY'

SEARCH INTERRUPTED

L7 QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

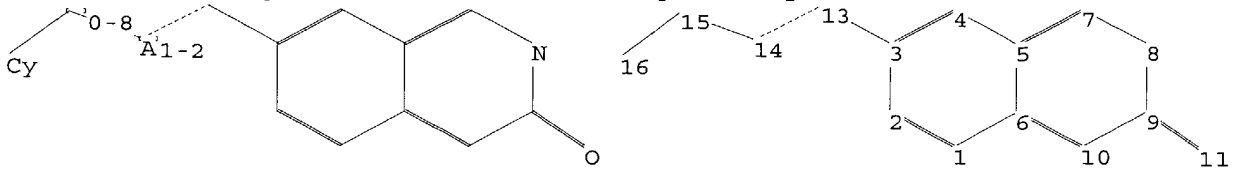
L8 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L9 SCREEN CREATED

=>

Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (ex 2).str



chain nodes :
11 13 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-13 9-11 13-14 14-15 15-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-11 13-14 14-15 15-16
exact bonds :
3-13
isolated ring systems :
containing 1 :

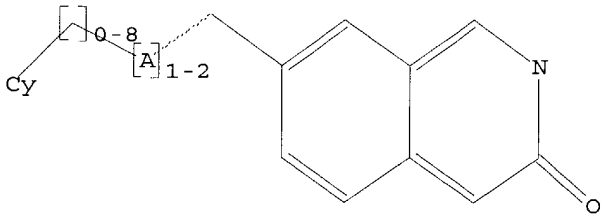
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom

L10 STRUCTURE UPLOADED

=> que L10 AND L8 NOT L9

L11 QUE L10 AND L8 NOT L9

=> d l11
L11 HAS NO ANSWERS
L8 SCR 1839
L9 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L10 STR



Structure attributes must be viewed using STN Express query preparation.
L11 QUE L10 AND L8 NOT L9

=> s l11 sss sam

SAMPLE SEARCH INITIATED 11:04:00 FILE 'REGISTRY'

SEARCH INTERRUPTED

L12 QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

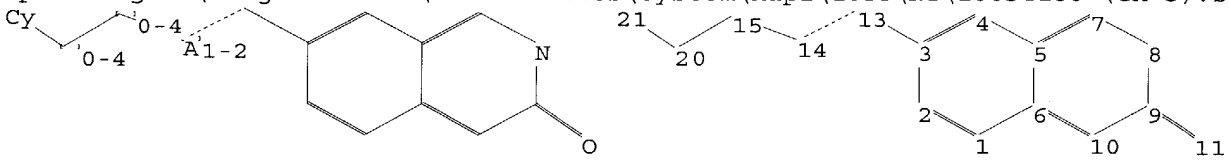
=> screen 1839

L13 SCREEN CREATED

=> screen 2026 OR 2016 OR 2039 OR 2040 OR 2045 OR 2047

L14 SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (ex 3).str



chain nodes :
11 13 14 15 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-13 9-11 13-14 14-15 15-20 20-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-11 13-14 14-15 20-21
exact bonds :
3-13 15-20
isolated ring systems :
containing 1 :

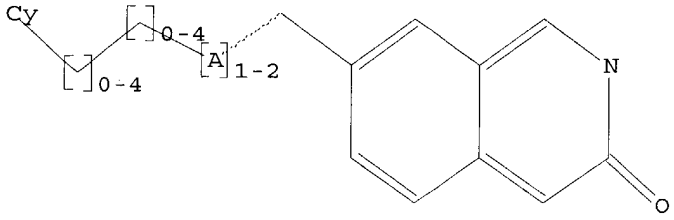
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:CLASS 15:CLASS 20:CLASS 21:Atom

L15 STRUCTURE UPLOADED

=> que L15 AND L13 NOT L14

L16 QUE L15 AND L13 NOT L14

=> d l16
L16 HAS NO ANSWERS
L13 SCR 1839
L14 SCR 2026 OR 2016 OR 2039 OR 2040 OR 2045 OR 2047
L15 STR



Structure attributes must be viewed using STN Express query preparation.
L16 QUE L15 AND L13 NOT L14

=> s l15 sss sam
SAMPLE SEARCH INITIATED 11:05:42 FILE 'REGISTRY'
SCREENING
SAMPLE SCREEN SEARCH COMPLETED - 5432 TO ITERATE

18.4% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.24

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 104222 TO 113058
PROJECTED ANSWERS: 0 TO 0

L17 0 SEA SSS SAM L15

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

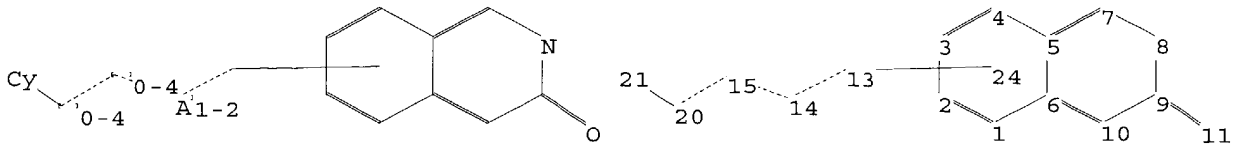
=> screen 1839

L18 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L19 SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (ex 4).str



chain nodes :
11 13 14 15 20 21
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
9-11 13-14 14-15 15-20 20-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 9-11 13-14 14-15 15-20
20-21
isolated ring systems :
containing 1 :

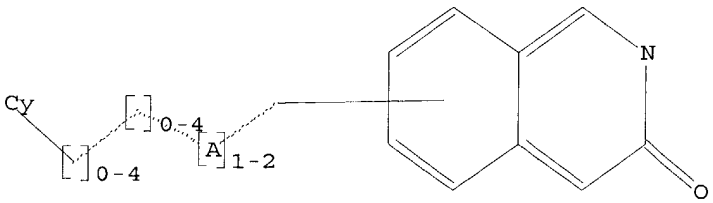
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 13:CLASS 14:CLASS 15:CLASS 20:CLASS 21:Atom 24:CLASS

L20 STRUCTURE UPLOADED

=> que L20 AND L18 NOT L19

L21 QUE L20 AND L18 NOT L19

=> d l21
L21 HAS NO ANSWERS
L18 SCR 1839
L19 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L20 STR



Structure attributes must be viewed using STN Express query preparation.
L21 QUE L20 AND L18 NOT L19

=> s l21 sss sam
SAMPLE SEARCH INITIATED 11:08:17 FILE 'REGISTRY'

```
SEARCH INTERRUPTED

L22  QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> s l17 sss ful
FULL SEARCH INITIATED 11:08:32 FILE 'REGISTRY'

SEARCH INTERRUPTED

L23  QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> d his

     (FILE 'HOME' ENTERED AT 11:01:21 ON 19 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 11:01:26 ON 19 MAR 2004
L1              SCREEN 1839
L2              SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L3              STRUCTURE UPLOADED
L4              QUE L3 AND L1 NOT L2
L5              QUE L3 AND L1 NOT L2
L6              QUE L3 AND L1 NOT L2
L7              QUE L3 AND L1 NOT L2
L8              SCREEN 1839
L9              SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L10             STRUCTURE UPLOADED
L11             QUE L10 AND L8 NOT L9
L12             QUE L10 AND L8 NOT L9
L13             SCREEN 1839
L14             SCREEN 2026 OR  2016 OR  2039 OR  2040 OR  2045 OR  2047
L15             STRUCTURE UPLOADED
L16             QUE L15 AND L13 NOT L14
L17           0 S L15 SSS SAM
L18             SCREEN 1839
L19             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L20             STRUCTURE UPLOADED
L21             QUE L20 AND L18 NOT L19
L22             QUE L20 AND L18 NOT L19
L23             QUE L15

=> s l15 sss ful
FULL SEARCH INITIATED 11:09:01 FILE 'REGISTRY'

SEARCH INTERRUPTED

L24  QUERY CREATED
If this message appears repeatedly, please notify the Help Desk.
Enter "HELP STN" for information on contacting the nearest STN Help
Desk by telephone or via SEND in the STNMAIL file.

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end
```

```
=> screen 1839

L25   SCREEN CREATED

=> screen 2026 OR  2016 OR  2039 OR  2040 OR  2045 OR  2047

L26   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10634180 (ex 3).str
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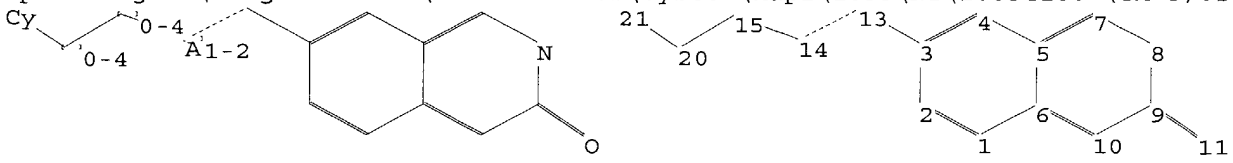


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chain nodes :
11  13  14  15  20  21
ring nodes :
1  2  3  4  5  6  7  8  9  10
chain bonds :
3-13  9-11  13-14  14-15  15-20  20-21
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-10  7-8  8-9  9-10  9-11  13-14  14-15  20-21
exact bonds :
3-13  15-20
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:Atom
11:CLASS  13:CLASS  14:CLASS  15:CLASS  20:CLASS  21:Atom



L27     STRUCTURE UPLOADED

=> que L27 AND L25 NOT L26

L28  QUE L27 AND L25 NOT L26

=> d l28
L28 HAS NO ANSWERS
L25             SCR 1839
L26             SCR 2026 OR 2016 OR 2039 OR 2040 OR 2045 OR 2047
L27             STR
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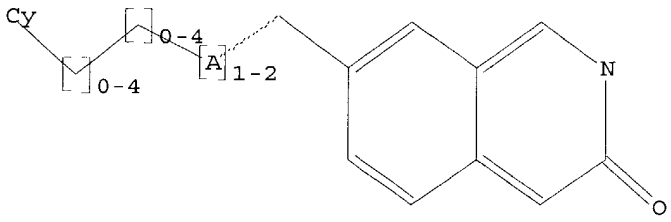


Structure attributes must be viewed using STN Express query preparation.
L28 QUE L27 AND L25 NOT L26

=> s l28 sss sam
SAMPLE SEARCH INITIATED 11:09:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5049 TO ITERATE

19.8% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 96720 TO 105240
PROJECTED ANSWERS: 0 TO 0

L29 0 SEA SSS SAM L27 AND L25 NOT L26

=> s l28 sss ful
FULL SEARCH INITIATED 11:10:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 99120 TO ITERATE

100.0% PROCESSED 99120 ITERATIONS 18 ANSWERS
SEARCH TIME: 00.00.04

L30 18 SEA SSS FUL L27 AND L25 NOT L26

=> => s l30
L31 1 L30

=> d bib,ab,hitstr

L31 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2004:142961 CAPLUS
DN 140:199211
TI 3-Isoquinolinone derivatives as matrix metalloproteinase inhibitors, particularly for MMP-13, and their preparation and use as antiarthritics
IN Bunker, Amy Mae; Sliskovic, Drago Robert
PA Warner-Lambert Company Llc, USA
SO PCT Int. Appl., 127 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

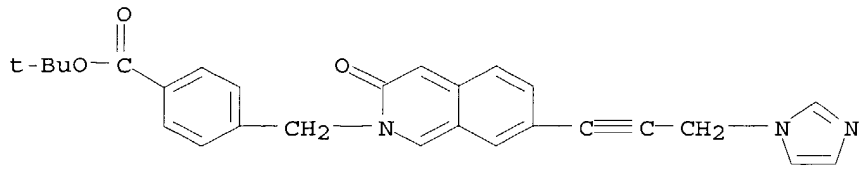
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004014378	A1	20040219	WO 2003-IB3508	20030803
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004038959	A1	20040226	US 2003-634180	20030805
PRAI US 2002-403062P	P	20020813		

AB The invention provides compds. I or pharmaceutically acceptable salts thereof [wherein: R1 = (un)substituted (bi/hetero)cycloalkylalkenyl, phenylalkenyl, naphthylalkenyl, Ph, naphthyl, hetero(bi)arylalkenyl, hetero(bi)aryl; Q = OC(O), C.tplbond.C, (un)substituted CH2C(O), OC(:NH), NHC(O), NHC(:S), SC(O), CH:CH, CH2C.tplbond.C, 2-oxopyrrolidine-1,n-diyl, etc.; R2 = H, alkyl, phenylalkenyl, naphthylalkenyl, hetero(bi)arylalkenyl, phenyl(oxy/thio/sulfinyl/sulfonyl)alkenyl; R3 = H, OH, alkoxy, (di)(alkyl)amino, (un)substituted alk(en/yn)yl, (hetero)cycloalkyl(alkenyl), phenyl(alkenyl), naphthyl(alkenyl); R4 = H, alkyl, NH2, OH, or halo; n = 0-3; W, X, Y = (independently) N or CR4]. I are selective MMP-13 inhibitors (no data), useful particularly for treatment of osteoarthritis and rheumatoid arthritis. The invention also provides pharmaceutical compns. comprising I, and the use of I as medicaments for treating diseases mediated by an MMP-13 enzyme. Claims include 18 specifically named compds., all 2H-isoquinolin-3-one derivs. Examples include 1 example with phys. data and 18 without data; the latter include prophetic examples of aza-, diaza-, and triaza-modified isoquinolinones. Formulation examples are also provided; several of these include co-formulations with COX-2 inhibitors, including valdecoxib or celecoxib. For instance, N-alkylation of 7-bromo-3-hydroxyisoquinoline by 4-(bromomethyl)benzoic acid tert-Bu ester, followed by CuI/Pd(PPh3)4-catalyzed alkynylation with PhCH2C.tplbond.CH, gave title compound II.

IT **662139-31-3P**, 4-[[7-[3-(Imidazol-1-yl)prop-1-ynyl]-3-oxo-2H-isoquinolin-2-yl]methyl]benzoic acid tert-butyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of isoquinolinone derivs. as selective MMP-13 inhibitors for use as antiarthritics)

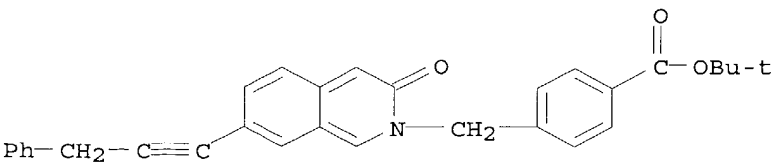
RN 662139-31-3 CAPLUS
CN Benzoic acid, 4-[[7-[3-(1H-imidazol-1-yl)-1-propynyl]-3-oxo-2(3H)-

isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

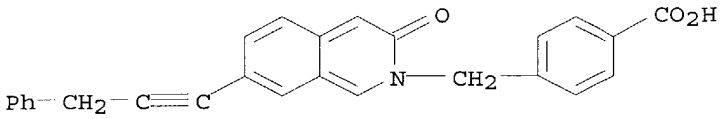


IT **662139-27-7P**, 4-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzoic acid tert-butyl ester **662139-28-8P**, 4-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzoic acid **662139-29-9P**, 7-(3-Phenylprop-1-ynyl)-2-(4-trifluoromethylbenzyl)-2H-isoquinolin-3-one **662139-30-2P**, 2-(3,5-Difluoro-4-hydroxybenzyl)-7-[3-(4H-[1,2,3]triazol-4-yl)prop-1-ynyl]-2H-isoquinolin-3-one **662139-32-4P**, 4-[[7-[3-(Imidazol-1-yl)prop-1-ynyl]-3-oxo-2H-isoquinolin-2-yl]methyl]benzoic acid **662139-33-5P**, 2-(3-Fluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-3-one **662139-34-6P**, 3-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzonitrile **662139-35-7P**, 4-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzenesulfonamide **662139-36-8P**, 4-[[3-Oxo-7-[3-([1,2,3]triazol-1-yl)prop-1-ynyl]-2H-isoquinolin-2-yl]methyl]benzoic acid tert-butyl ester **662139-37-9P**, 4-[[3-Oxo-7-[3-([1,2,3]triazol-1-yl)prop-1-ynyl]-2H-isoquinolin-2-yl]methyl]benzoic acid **662139-38-0P**, 4-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzoic acid methyl ester **662139-39-1P**, 3-[[3-Oxo-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-2-yl]methyl]benzoic acid methyl ester **662139-40-4P**, 2-(4-Fluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-3-one **662139-41-5P**, 7-(3-Phenylprop-1-ynyl)-2-(3-trifluoromethylbenzyl)-2H-isoquinolin-3-one **662139-42-6P**, 2-(3-Chlorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-3-one **662139-43-7P**, 2-(3,4-Difluorobenzyl)-7-(3-phenylprop-1-ynyl)-2H-isoquinolin-3-one **662139-44-8P**, 4-[[3-Oxo-7-[3-([1,2,4]triazol-1-yl)prop-1-ynyl]-2H-isoquinolin-2-yl]methyl]benzoic acid tert-butyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of isoquinolinone derivs. as selective MMP-13 inhibitors for use as antiarthritics)

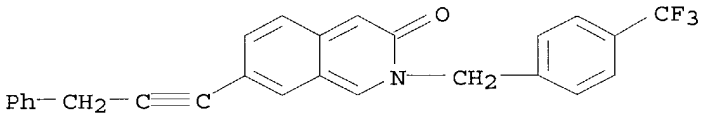
RN 662139-27-7 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



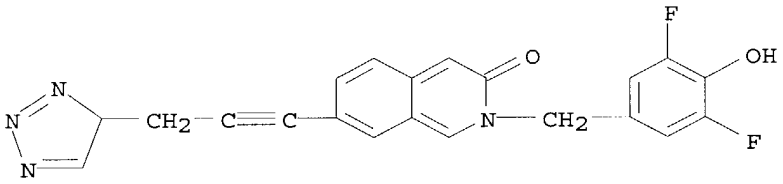
RN 662139-28-8 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)



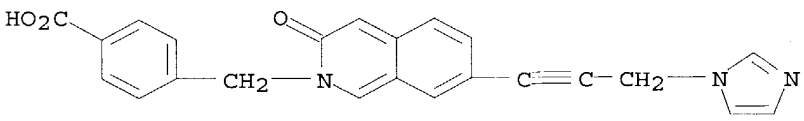
RN 662139-29-9 CAPLUS
CN 3(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



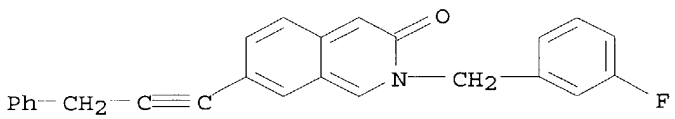
RN 662139-30-2 CAPLUS
CN 3(2H)-Isoquinolinone, 2-[(3,5-difluoro-4-hydroxyphenyl)methyl]-7-[3-(4H-1,2,3-triazol-4-yl)-1-propynyl]- (9CI) (CA INDEX NAME)



RN 662139-32-4 CAPLUS
CN Benzoic acid, 4-[[7-[3-(1H-imidazol-1-yl)-1-propynyl]-3-oxo-2(3H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)

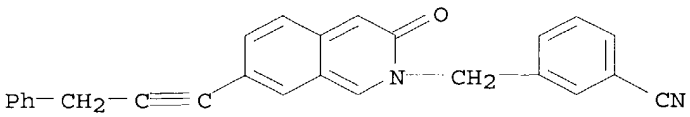


RN 662139-33-5 CAPLUS
CN 3(2H)-Isoquinolinone, 2-[(3-fluorophenyl)methyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

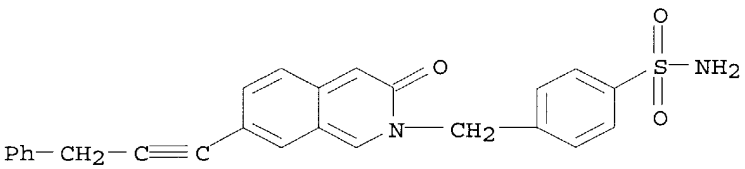


RN 662139-34-6 CAPLUS

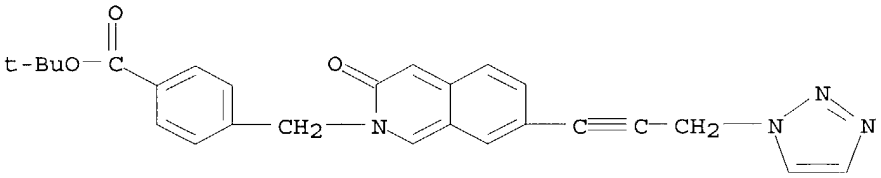
CN Benzonitrile, 3-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)



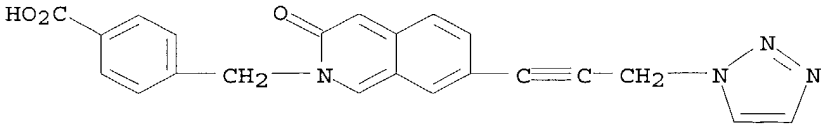
RN 662139-35-7 CAPLUS
CN Benzenesulfonamide, 4-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)



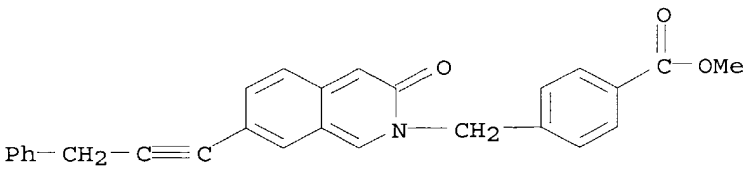
RN 662139-36-8 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-[3-(1H-1,2,3-triazol-1-yl)-1-propynyl]-2(3H)-isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



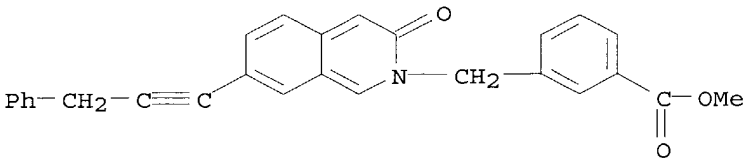
RN 662139-37-9 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-[3-(1H-1,2,3-triazol-1-yl)-1-propynyl]-2(3H)-isoquinolinyl]methyl]- (9CI) (CA INDEX NAME)



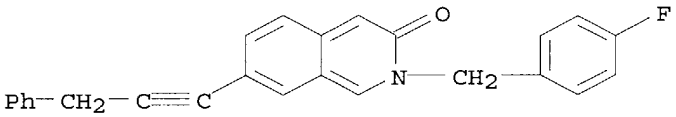
RN 662139-38-0 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



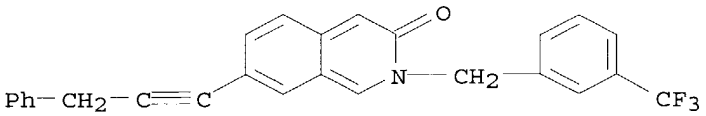
RN 662139-39-1 CAPLUS
CN Benzoic acid, 3-[[3-oxo-7-(3-phenyl-1-propynyl)-2(3H)-isoquinolinyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



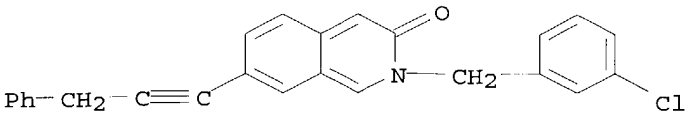
RN 662139-40-4 CAPLUS
CN 3(2H)-Isoquinolinone, 2-[(4-fluorophenyl)methyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)



RN 662139-41-5 CAPLUS
CN 3(2H)-Isoquinolinone, 7-(3-phenyl-1-propynyl)-2-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

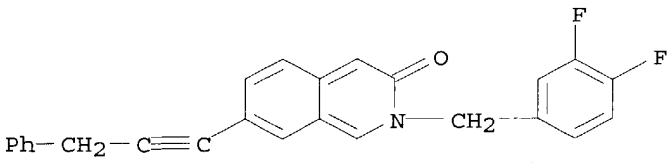


RN 662139-42-6 CAPLUS
CN 3(2H)-Isoquinolinone, 2-[(3-chlorophenyl)methyl]-7-(3-phenyl-1-propynyl)-(9CI) (CA INDEX NAME)

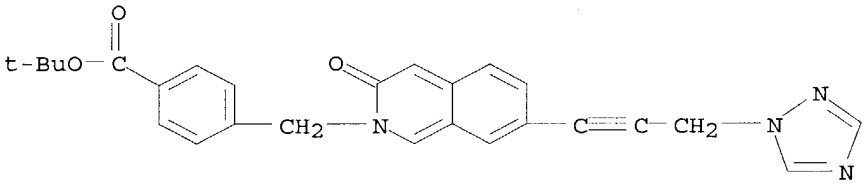


RN 662139-43-7 CAPLUS

CN 3(2H)-Isoquinolinone, 2-[(3,4-difluorophenyl)methyl]-7-(3-phenyl-1-propynyl)- (9CI) (CA INDEX NAME)



RN 662139-44-8 CAPLUS
CN Benzoic acid, 4-[[3-oxo-7-[3-(1H-1,2,4-triazol-1-yl)-1-propynyl]-2(3H)-isoquinolinyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

WO 99/64400
EP 1069110
US 2002 086890

```
=> => d his

     (FILE 'HOME' ENTERED AT 11:01:21 ON 19 MAR 2004)

     FILE 'REGISTRY' ENTERED AT 11:01:26 ON 19 MAR 2004
L1               SCREEN 1839
L2               SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L3               STRUCTURE UPLOADED
L4               QUE L3 AND L1 NOT L2
L5               QUE L3 AND L1 NOT L2
L6               QUE L3 AND L1 NOT L2
L7               QUE L3 AND L1 NOT L2
L8               SCREEN 1839
L9               SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L10              STRUCTURE UPLOADED
L11              QUE L10 AND L8 NOT L9
L12              QUE L10 AND L8 NOT L9
L13              SCREEN 1839
L14              SCREEN 2026 OR  2016 OR  2039 OR  2040 OR  2045 OR  2047
L15              STRUCTURE UPLOADED
L16              QUE L15 AND L13 NOT L14
L17            0 S L15 SSS SAM
L18              SCREEN 1839
L19              SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L20              STRUCTURE UPLOADED
L21              QUE L20 AND L18 NOT L19
L22              QUE L20 AND L18 NOT L19
L23              QUE L15
L24              QUE L15
L25              SCREEN 1839
L26              SCREEN 2026 OR  2016 OR  2039 OR  2040 OR  2045 OR  2047
L27              STRUCTURE UPLOADED
L28              QUE L27 AND L25 NOT L26
L29            0 S L28 SSS SAM
L30           18 S L28 SSS FUL

     FILE 'CAPLUS' ENTERED AT 11:10:42 ON 19 MAR 2004
L31            1 S L30

     FILE 'CAOLD' ENTERED AT 11:11:09 ON 19 MAR 2004

=> s l30
L32            0 L30

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.42     167.12

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00      -0.69

STN INTERNATIONAL LOGOFF AT 11:11:40 ON 19 MAR 2004
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